# A new two-pole approximation in the Hubbard model. Metal-insulator transition

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Two-pole approaches in the Hubbard model [1] and the Hubbard bands conception (being the consequence of a two-pole approximation) have been useful for understanding of the peculiarities of electric and magnetic properties of narrow-band materials [1]-[13]. However within the framework of two-pole approaches there are series of issues, in particular the problem of metal-insulator transition description.

In this paper a new two-pole approximation, which allows to describe the transition from an insulating state to a metallic one at increase of bandwidth, and also the observable in some compounds transition from a metalic state to an insulating one with increasing temperature, is presented.

Let us take the operators of creation and destruction of an electron with spin $\sigma$ ($\sigma = \downarrow, \uparrow$) on $i$-site in the form:

$$a_{i\sigma}^+ = d_{i\sigma}^+ + h_{i\sigma}, \quad a_{i\sigma} = d_{i\sigma} + h_{i\sigma}^+, \tag{1}$$

where $d_{i\sigma}^+ = a_{i\sigma}^+ n_{i\bar{\sigma}}$, $d_{i\sigma} = a_{i\sigma} n_{i\bar{\sigma}}$, $h_{i\sigma}^+ = a_{i\sigma}(1 - n_{i\bar{\sigma}})$, $h_{i\sigma} = a_{i\sigma}^+(1 - n_{i\bar{\sigma}})$, and $\bar{\sigma}$ denotes the projection of electron spin opposite to $\sigma$. Between the $d$-$h$-operators and Hubbard $X$-operators [14] direct relations exist [15]. The Hubbard Hamiltonian [1] in terms of the $d$-$h$-operators is written as

$$H = H_0 + H_1 + H_1', \tag{2}$$

$$H_0 = -\frac{\mu}{2} \sum_{i\sigma} \left( d_{i\sigma}^+ d_{i\sigma} + h_{i\sigma} h_{i\sigma}^+ \right) + \frac{U}{2} \sum_{i\sigma} d_{i\sigma}^+ d_{i\sigma}, \tag{3}$$

$$H_1 = t \sum_{ij\sigma, i\neq j} \left( d_{i\sigma}^+ d_{j\sigma} - h_{i\sigma}^+ h_{j\sigma} \right), \quad H_1' = t \sum_{ij\sigma, i\neq j} \left( d_{i\sigma}^+ h_{j\sigma}^+ + h.c. \right), \tag{4}$$

where $\mu$ is the chemical potential; $U$ is the intra-atomic Coulomb repulsion; $t$ is the nearest-neighbor hopping integral. $H_0$ describes system in the atomic limit, $H_1$ describes electron hoppings between doubly occupied sites (with two electrons of opposite spins - doublons) and single occupied sites (the first sum in $H_1$) and electron hoppings between single occupied sites and empty sites (holes) (the second sum in $H_1$). $H_1'$ describes "hybridization" between the "h-band" and "d-band" (the processes of pair creation and annihilation of holes and doublons). The structure of the Hamiltonian originates the approximation given below.

The Green functions $\langle\langle d_{p\uparrow}|d_{s\uparrow}^+\rangle\rangle$ and $\langle\langle h_{p\uparrow}^+|d_{s\uparrow}^+\rangle\rangle$ satisfy the equations:

$$(E + \mu - U)\langle\langle d_{p\uparrow}|d_{s\uparrow}^+\rangle\rangle = \frac{n_\uparrow}{2\pi}\delta_{ps} + \langle\langle[d_{p\uparrow}, H_1]_-|d_{s\uparrow}^+\rangle\rangle$$

$$+t\sum_i \langle\langle(h_{p\downarrow}h_{p\uparrow}^+ h_{i\downarrow}^+ - h_{p\uparrow}^+ d_{p\downarrow}d_{i\downarrow}^+ - n_{p\downarrow}h_{i\uparrow}^+)|d_{s\uparrow}^+\rangle\rangle, \tag{5}$$

$$(E + \mu)\langle\langle h_{p\uparrow}^+|d_{s\uparrow}^+\rangle\rangle = \langle\langle[h_{p\uparrow}^+, H_1]_-|d_{s\uparrow}^+\rangle\rangle$$

$$+t\sum_{i}\langle\langle(h_{p\downarrow}h_{p\uparrow}^{+}d_{i\downarrow}-h_{p\uparrow}^{+}d_{p\downarrow}h_{i\downarrow}-(1-n_{p\downarrow})d_{i\uparrow})|d_{s\uparrow}^{+}\rangle\rangle, \tag{6}$$

with $n_{p\sigma}=a_{p\sigma}^{+}a_{p\sigma}$, $n_{\sigma}=\langle n_{p\sigma}\rangle$ and $[A,B]_{-}=AB-BA$. To obtain the closed system of equations for the Green functions $\langle\langle d_{p\uparrow}|d_{s\uparrow}^{+}\rangle\rangle$ and $\langle\langle h_{p\uparrow}^{+}|d_{s\uparrow}^{+}\rangle\rangle$ we suppose

$$\langle\langle[d_{p\uparrow},H_{1}]_{-}|d_{s\uparrow}^{+}\rangle\rangle=\sum_{j}\varepsilon(pj)\langle\langle d_{j\uparrow}|d_{s\uparrow}^{+}\rangle\rangle, \tag{7}$$

$$\langle\langle[h_{p\uparrow}^{+},H_{1}]_{-}|d_{s\uparrow}^{+}\rangle\rangle=\sum_{j}\varepsilon_{1}(pj)\langle\langle h_{j\uparrow}|d_{s\uparrow}^{+}\rangle\rangle, \tag{8}$$

where $\varepsilon(pj)$, $\varepsilon_{1}(pj)$ are the non-operator expressions which are calculated by the method decribed in Ref. [13]. At electron concentration $n=1$ (this is the important situation to study metal-insulator transition) in a paramagnetic state ($n_{\uparrow}=n_{\downarrow}$) we have $\varepsilon(pj)=\varepsilon_{1}(pj)=(1-2c)t$, with $c$ being the concentration of polar states (holes or doublons). For the model Hamiltonian $H_{0}+H_{1}$ this approximation leads to the criterion of metal-insulator transition $(U/2w)_{cr}=1$ reproducing the exact result of Ref. [16].

Among the Green function originated from the expressions $\langle\langle[d_{p\uparrow},H_{1}']_{-}|d_{s\uparrow}^{+}\rangle\rangle$ and $\langle\langle[h_{p\uparrow}^{+},H_{1}']_{-}|d_{s\uparrow}^{+}\rangle\rangle$ we take into account the "diagonal" Green function only. The decoupling procedure of these Green functions is made by means of the mean-field approximation:

$$\langle\langle n_{p\downarrow}h_{i\uparrow}^{+}|d_{s\uparrow}^{+}\rangle\rangle\simeq 1/2\langle\langle h_{i\uparrow}^{+}|d_{s\uparrow}^{+}\rangle\rangle, \qquad \langle\langle(1-n_{p\downarrow})d_{i\uparrow})|d_{s\uparrow}^{+}\rangle\rangle\simeq 1/2\langle\langle d_{i\uparrow}^{+}|d_{s\uparrow}^{+}\rangle\rangle; \tag{9}$$

by making these approximations we neglect the processes describing the "inter-band" hoppings of electrons which are connected with spin turning over and "inter-band" hoppings with creation or annihilation of two electrons on the same site.

Finally, in **k**-representation one-electron Green function is

$$\langle\langle a_{p\uparrow}|a_{s\uparrow}^{+}\rangle\rangle_{\mathbf{k}}=\frac{1}{4\pi}\left(\frac{A_{\mathbf{k}}}{E-E_{1}(\mathbf{k})}+\frac{B_{\mathbf{k}}}{E-E_{2}(\mathbf{k})}\right), \tag{10}$$

$$A_{\mathbf{k}}=1-\frac{t(\mathbf{k})}{\sqrt{U^{2}+t^{2}(\mathbf{k})}}, \quad B_{\mathbf{k}}=1+\frac{t(\mathbf{k})}{\sqrt{U^{2}+t^{2}(\mathbf{k})}}, \tag{11}$$

$$E_{1,2}(\mathbf{k})=(1-2c)t(\mathbf{k})\mp\frac{1}{2}\sqrt{U^{2}+t^{2}(\mathbf{k})}, \tag{12}$$

where $t(\mathbf{k})$ is the hopping integral in **k**-representation; $E_{1}(\mathbf{k})$ is the quasiparticle energy spectrum in the lower Hubbard band ($h$-band), $E_{2}(\mathbf{k})$ is the quasiparticle energy spectrum in the upper Hubbard band ($d$-band). One-electron Green function (10) and energy spectrum (12) are exact in the atomic and band limits.

The peculiarity of energy spectrum (12) is the dependence on polar states concentration (and on temperature), that differs it from the two-pole approximations of Hubbard [1], and Ikeda, Larsen, Mattuck [4]. A distinction of the proposed approximation from the approximations based on the ideology of Roth [3] (in this connection see also Refs. [7]-[11]) is, first of all, ability of the proposed approximation to describe metal-insulator transition. Spectrum (12) differs also from the spectrum earlier obtained by the author [13] by presence of term $\sqrt{U^{2}+t^{2}(\mathbf{k})}$ instead of the expression $\sqrt{U^{2}+4c^{2}t^{2}(\mathbf{k})}$ obtained in Ref. [13]. This leads to series of the distinctions of results of this work from the results of work [13] ($c(U/w)$– dependence, the condition of metal-insulator transition); for doped Mott-Hubbard materials, when electron concentration $n\neq 1$, and we can restrict ourselves to consideration one of two Hubbard's bands, approach of Ref. [13] and proposed in this work approach are equivalent.

The concentration of polar states is calculated with the help of the Green function

$$\langle\langle d_{p\uparrow}|d_{s\uparrow}^{+}\rangle\rangle_{\mathbf{k}} = \frac{1}{8\pi}\left(\frac{C_{\mathbf{k}}}{E - E_1(\mathbf{k})} + \frac{D_{\mathbf{k}}}{E - E_2(\mathbf{k})}\right), \tag{13}$$

$$C_{\mathbf{k}} = 1 - \frac{U}{\sqrt{U^2 + t^2(\mathbf{k})}}, \quad D_{\mathbf{k}} = 1 + \frac{U}{\sqrt{U^2 + t^2(\mathbf{k})}}. \tag{14}$$

At $T = 0$ we have

$$c = \frac{1}{4} + \frac{U}{8w}\ln\frac{1 - 4c}{3 - 4c} \tag{15}$$

if $U/2w \le (U/2w)_{cr}$ with $(U/2w)_{cr} = 0.836$ ($w = z|t|$, $z$ is the number of nearest neighbors to a site); for $U/2w > (U/2w)_{cr}$ the concentration of polar states is

$$c = \frac{1}{4} + \frac{U}{8w}\ln\frac{-w + \sqrt{U^2 + w^2}}{w + \sqrt{U^2 + w^2}}. \tag{16}$$

Expression (12) describes the vanishing of energy gap in the spectrum of paramagnetic insulator at increasing $w$ (under pressure). Really, the energy gap width (difference of energies between bottom of the upper and top of the lower Hubbard bands)

$$\Delta E = -2(1 - 2c)w + \sqrt{U^2 + w^2}. \tag{17}$$

vanishes when the condition $(U/2w)_{cr} = 0.836$ is satisfied. This value is close to the result of "Hubbard-III" approximation [17]. It is important to note that in the point of gap disappearance we have $c \ne 0$.

Energy gap (17) is temperature dependent. This allows to explain observed in some narrow-band materials transition from a metallic to an insulating state with increasing temperature (see, for example [6]).

Above we have considered the case of a paramagnetic narrow-band material at half-filling ($n = 1$). It is interesting to study non-halffilled case ($n \ne 1$); here the energy spectrum can be essentially modified by the spin-dependent (in general case) shifts of the Hubbard band centers (on the analogy with the Harris and Lange result [2]). This case (which is important to study ferromagnetism in narrow energy bands) will be considered in subsequent paper (as well as the problem of antiferromagnetism).

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